

# ON THE WIDOM–ROWLINSON OCCUPANCY FRACTION IN REGULAR GRAPHS

EMMA COHEN, WILL PERKINS, PRASAD TETALI

**ABSTRACT.** We consider the Widom–Rowlinson model of two types of interacting particles on  $d$ -regular graphs. We prove a tight upper bound on the occupancy fraction, the expected fraction of vertices occupied by a particle under a random configuration from the model. The upper bound is achieved uniquely by unions of complete graphs on  $d + 1$  vertices,  $K_{d+1}$ ’s. As a corollary we find that  $K_{d+1}$  also maximises the normalised partition function of the Widom–Rowlinson model over the class of  $d$ -regular graphs. A special case of this shows that the normalised number of homomorphisms from any  $d$ -regular graph  $G$  to the graph  $H_{\text{WR}}$ , a path on three vertices with a loop on each vertex, is maximised by  $K_{d+1}$ . This proves a conjecture of Galvin.

## 1. THE WIDOM–ROWLINSON MODEL

A *Widom–Rowlinson assignment* or *configuration* on a graph  $G$  is a map  $\chi : V(G) \rightarrow \{0, 1, 2\}$  so that 1 and 2 are not assigned to neighbouring vertices, or in other words, a graph homomorphism from  $G$  to the graph  $H_{\text{WR}}$  consisting of a path on 3 vertices with a loop on each vertex (the middle vertex represents the label 0). Call the set of all such assignments  $\Omega(G)$ . The *Widom–Rowlinson model* on  $G$  is a probability distribution over  $\Omega(G)$  parameterised by  $\lambda \in (0, \infty)$ , given by:

$$\mathbb{P}[\chi] = \frac{\lambda^{X_1(\chi) + X_2(\chi)}}{P_G(\lambda)},$$

where  $X_i(\chi)$  is the number of vertices coloured  $i$  under  $\chi$ , and

$$P_G(\lambda) = \sum_{\chi \in \Omega(G)} \lambda^{X_1(\chi) + X_2(\chi)}$$

is the *partition function*. Evaluating  $P_G(\lambda)$  at  $\lambda = 1$  counts the number of homomorphisms from  $G$  to  $H_{\text{WR}}$ . We think of vertices assigned 1 and 2 as “coloured” and those assigned 0 as “uncoloured” (see Figure 1).

The Widom–Rowlinson model was introduced by Widom and Rowlinson in 1970 [13], as a model of two types of interacting particles with a hard-core exclusion between particles of different types: colour 1 and 2 represent particles of each type and colour 0 represents an unoccupied site. The model has been studied both on lattices [9] and in the continuum [11, 2] and is known to exhibit a phase transition in both cases.

The Widom–Rowlinson model is one case of a general random model: that of choosing a random homomorphism from a large graph  $G$  to a fixed graph  $H$ . In the Widom–Rowlinson case, we take  $H = H_{\text{WR}}$ . Another notable case is  $H_{\text{ind}}$ , an edge between two vertices,

---

2010 *Mathematics Subject Classification.* 05C60, 05C35, 82B20.

Research of the first and the last authors is supported in part by the NSF grant DMS-1407657.

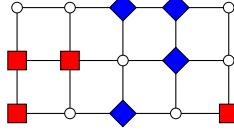


FIGURE 1. A configuration for the Widom–Rowlinson model on a grid. Vertices mapping to 1 and 2 are shown as squares and diamonds, respectively (corresponding to Figure 2).

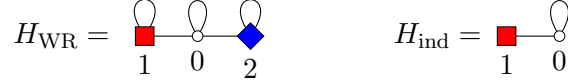


FIGURE 2. The target graphs for the Widom–Rowlinson model and the hard-core model.

one of which has a loop (see Figure 2). Homomorphisms from  $G$  to  $H_{\text{ind}}$  are exactly the independent sets of  $G$ , and the partition function of the hard-core model is the sum of  $\lambda^{|I|}$  over all independent sets  $I$ . An overview of the connections between statistical physics models with hard constraints, graph homomorphisms, and combinatorics can be found in [1].

For every such model, there is an associated extremal problem. Denote by  $\text{hom}(G, H)$  the number of homomorphisms from  $G$  to  $H$ . Then we can ask which graph  $G$  from a class of graphs  $\mathcal{G}$  maximises  $\text{hom}(G, H)$ , or if we wish to compare graphs on different numbers of vertices, ask which graph maximises the scaled quantity  $\text{hom}(G, H)^{1/|V(G)|}$ .

Kahn [8] proved that for any  $d$ -regular, bipartite graph  $G$ ,

$$(1) \quad \text{hom}(G, H_{\text{ind}}) \leq \text{hom}(K_{d,d}, H_{\text{ind}})^{|V(G)|/2d},$$

where  $K_{d,d}$  is the complete  $d$ -regular bipartite graph. Equality holds in (1) if  $G$  is  $K_{d,d}$  or a union of  $K_{d,d}$ 's. In other words, unions of  $K_{d,d}$ 's maximise the total number of independent sets over all  $d$ -regular, bipartite graphs on a fixed number of vertices.

In a broad generalisation of Kahn's result, Galvin and Tetali [7] showed that in fact, (1) holds for all  $d$ -regular, bipartite  $G$  and *all* target graphs  $H$  (including, for example,  $H_{\text{WR}}$ ). And using a cloning construction and a limiting argument, they showed that in fact the partition function of such models (a weighted count of homomorphisms) is maximised by  $K_{d,d}$ ; for example, for a  $d$ -regular, bipartite  $G$ ,

$$(2) \quad P_G(\lambda) \leq P_{K_{d,d}}(\lambda)^{|V(G)|/2d},$$

where  $P_G(\lambda)$  is the Widom–Rowlinson partition function defined above or the independence polynomial of a graph. Note that the case  $\lambda = 1$  is the counting result.

There is no such sweeping statement for the class of all  $d$ -regular graphs with the bipartiteness restriction removed. In [14] and [15], Zhao showed that the bipartiteness restriction on  $G$  in (1) and (2) can be removed for some class of graphs  $H$ , including  $H_{\text{ind}}$ . But such an extension is not possible for all graphs  $H$ ; for example,  $K_{d+1}$  has more homomorphisms to  $H_{\text{WR}}$  than does  $K_{d,d}$  (after normalising for the different numbers of vertices). In fact Galvin conjectured the following:

**Conjecture 1** (Galvin [5, 6]). *Let  $G$  be a any  $d$ -regular graph. Then*

$$\text{hom}(G, H_{WR}) \leq \text{hom}(K_{d+1}, H_{WR})^{|V(G)|/(d+1)}.$$

The more general Conjecture 1.1 of [5] that the maximising  $G$  for any  $H$  is either  $K_{d,d}$  or  $K_{d+1}$  has been disproved by Sernau [12].

The above theorems of Kahn and Galvin and Tetali are based on the *entropy method* (see [10] and [6] for a survey), but in this context bipartiteness seems essential for the effectiveness of the method. We will approach the problem differently, using the *occupancy method* of [3].

We first define the *occupancy fraction*  $\alpha_G(\lambda)$  to be the expected fraction of vertices which receive a (nonzero) colour in the Widom–Rowlinson model:

$$\alpha_G(\lambda) = \frac{\mathbb{E}[X_1 + X_2]}{|V(G)|},$$

where  $X_i$  is the number of vertices coloured  $i$  by the random assignment  $\chi$ . A calculation shows that  $\alpha_G(\lambda)$  is in fact the scaled logarithmic derivative of the partition function:

$$(3) \quad \alpha_G(\lambda) = \frac{\lambda}{|V(G)|} \cdot \frac{P'_G(\lambda)}{P_G(\lambda)} = \frac{\lambda \cdot (\log P_G(\lambda))'}{|V(G)|}.$$

Our main result is that for any  $\lambda$ ,  $\alpha_G(\lambda)$  is maximised over all  $d$ -regular graphs  $G$  by  $K_{d+1}$ .

**Theorem 2.** *Let  $G$  be any  $d$ -regular graph and  $\lambda > 0$ . Then*

$$\alpha_G(\lambda) \leq \alpha_{K_{d+1}}(\lambda)$$

*with equality if and only if  $G$  is a union of  $K_{d+1}$ 's.*

We will prove this by introducing local constraints on random configurations induced by the Widom–Rowlinson model on a  $d$ -regular graph  $G$ , then solving a linear programming relaxation of the optimisation problem over all  $d$ -regular graphs.

Theorem 2 implies maximality of the normalised partition function:

**Corollary 3.** *Let  $G$  be a  $d$ -regular graph and  $\lambda > 0$ . Then*

$$\frac{1}{|V(G)|} \log P_G(\lambda) \leq \frac{1}{d+1} \log P_{K_{d+1}}(\lambda),$$

*or equivalently,*

$$P_G(\lambda) \leq P_{K_{d+1}}(\lambda)^{|V(G)|/(d+1)},$$

*with equality if and only if  $G$  is a union of  $K_{d+1}$ 's.*

The quantity  $\frac{1}{|V(G)|} \log P_G(\lambda)$  is known in statistical physics as the *free energy per unit volume*. Corollary 3 follows from Theorem 2 as follows:  $\frac{1}{|V(G)|} \log P_G(0) = 0$  for any  $G$ , and so

$$\begin{aligned} \frac{1}{|V(G)|} \log P_G(\lambda) &= \frac{1}{|V(G)|} \int_0^\lambda (\log P_G(t))' dt \\ &\leq \frac{1}{d+1} \int_0^\lambda (\log P_{K_{d+1}}(t))' dt = \frac{1}{d+1} \log P_{K_{d+1}}(\lambda) \end{aligned}$$

where the inequality follows from Theorem 2 and (3). Exponentiating both sides gives Corollary 3.

By taking  $\lambda = 1$  in Corollary 3, we get the counting result:

**Corollary 4.** *For all  $d$ -regular  $G$ ,*

$$\text{hom}(G, H_{WR}) \leq \text{hom}(K_{d+1}, H_{WR})^{|V(G)|/(d+1)}$$

*with equality if and only if  $G$  is a union of  $K_{d+1}$ 's.*

This proves Conjecture 1.

**Discussion and related work.** The method we use is more probabilistic than the entropy method in the sense that Theorem 2 gives information about an observable of the model; in some statistical physics models, the analogue of  $\alpha_G(\lambda)$  would be called the *mean magnetisation*. We also work directly in the statistical physics model, instead of counting homomorphisms.

Davies, Jenssen, Perkins, and Roberts [3] applied the occupancy method to two central models in statistical physics: the hard-core model of a random independent set described above, and the monomer-dimer model of a randomly chosen matching from a graph  $G$ . In both cases they showed that  $K_{d,d}$  maximises the occupancy fraction over all  $d$ -regular graphs. In the case of independent sets this gives a strengthening of the results of Kahn, Galvin and Tetali, and Zhao, while for matchings, it was not known previously that unions of  $K_{d,d}$  maximises the partition function or the total number of matchings.

The idea of calculating the log partition function by integrating a partial derivative is not new of course; see for example, the interpolation scheme of Dembo, Montanari, and Sun [4] in the context of Gibbs distributions on locally tree-like graphs. The method is powerful because it reduces the computation of a very global quantity,  $P_G(\lambda)$ , to that of a locally estimable quantity,  $\alpha_G(\lambda)$ .

Some partial results towards the Widom–Rowlinson counting problem were obtained by Galvin [5], who showed that a graph with more homomorphisms than a union of  $K_{d+1}$ 's must be close in a specific sense to a union of  $K_{d+1}$ 's.

## 2. PROOF OF THEOREM 2

**2.1. Preliminaries.** To prove Theorem 2, we will use the following experiment: for a  $d$ -regular graph  $G$ , we first draw a random  $\chi$  from the Widom–Rowlinson model, then select a vertex  $v$  uniformly at random from  $V(G)$ . We then write our objective function, the occupancy fraction, in terms of local probabilities with respect to this experiment, and add constraints on the local probabilities that must hold for all  $G$ . We then relax the optimisation problem to all distributions satisfying the local constraints, and optimise using linear programming.

Fix  $d$  and  $\lambda$ . Define a *configuration with boundary conditions*  $C = (H, \mathcal{L})$  to be a graph  $H$  on  $d$  vertices with family of lists  $\mathcal{L} = \{L_u\}_{u \in H}$ , where each  $L_u \subseteq \{1, 2\}$  is a set of allowed colours for the vertex  $u$ . Here  $H$  represents the neighbourhood structure of a vertex  $v \in V(G)$  and the colour lists  $L_u$  represent the colours permitted to neighbours of  $v$ , given an assignment  $\chi$  on the vertices outside of  $N(v) \cup \{v\}$ . (See Figure 3.) Denote by  $\mathcal{C}$  the set of all possible configurations with boundary conditions in any  $d$ -regular graph.

We now pick the assignment  $\chi$  at random from the Widom–Rowlinson model on a fixed  $d$ -regular graph  $G$ , pick a vertex  $v$  uniformly at random from  $V(G)$ , and consider the probability distribution induced on  $\mathcal{C}$ .

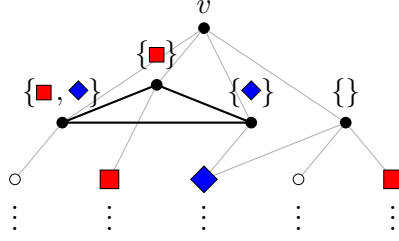


FIGURE 3. An example configuration with boundary conditions based on a colouring  $\chi$ . The graph  $H$  consists of the four neighbours of  $v$  along with the black edges, and the list  $L_u$  is shown above each vertex  $u$  of  $H$ . The colours assigned by  $\chi$  to  $v$  and its neighbours are immaterial and so are not shown.

For example, if  $G = K_{d+1}$  then with probability 1 the random configuration  $C$  is  $H = K_d$  with  $L_u = \{1, 2\}$  for all  $u \in V(H)$ . If  $G = K_{d,d}$  then  $H$  is always  $d$  isolated vertices and the colour lists can be any (possibly empty) subset of  $\{1, 2\}$ , but the lists must be the same for all  $u \in V(H)$ .

For a configuration  $C = (H, \mathbf{L})$ , define

$$\alpha_i^v(C) = \mathbb{P}[\chi(v) = i \mid C]$$

$$\alpha_i^u(C) = \frac{1}{d} \sum_{u \in V(H)} \mathbb{P}[\chi(u) = i \mid C],$$

where the probability is over the Widom–Rowlinson model on  $G$  given the boundary conditions  $\mathcal{L}$ . Note that the spatial Markov property of the model means that these probabilities are “local” in the sense that they can be computed knowing only  $C$ . Let  $\alpha^v(C) = \alpha_1^v(C) + \alpha_2^v(C)$  and  $\alpha^u(C) = \alpha_1^u(C) + \alpha_2^u(C)$ . Then we have

$$(4) \quad \alpha_G(\lambda) = \frac{1}{|V(G)|} \sum_{v \in V(G)} \mathbb{P}[\chi(v) \in \{1, 2\}] = \mathbb{E}_C[\alpha^v(C)]$$

$$= \frac{1}{d} \frac{1}{|V(G)|} \sum_{v \in V(G)} \sum_{u \sim v} \mathbb{P}[\chi(u) \in \{1, 2\}] = \mathbb{E}_C[\alpha^u(C)],$$

where the expectations are over the probability distribution induced on  $\mathcal{C}$  by our experiment of drawing  $\chi$  from the model and  $v$  uniformly at random from  $V(G)$ , and the last sum is over all neighbours of  $v$  in  $G$ . Equality of the two expressions for  $\alpha$  follows since sampling a uniform neighbour of a uniform vertex in a regular graph is equivalent to sampling a uniform vertex. We will show that this expectation is maximised when the graph  $G$  is  $K_{d+1}$ .

We can in fact write explicit formulae for  $\alpha^v(C)$  and  $\alpha^u(C)$ . For a configuration  $C = (H, \mathbf{L})$ , let  $P_C^{(0)}(\lambda)$  be the total weight of colourings of  $H$  satisfying the boundary conditions given by the lists  $\mathbf{L}$  (corresponding to the partition function for the neighbourhood of  $v$  conditioned on  $\chi(v) = 0$ ). Also, write  $P_C^{(i)}(\lambda)$  for the total weight of colourings of  $H$  satisfying the boundary conditions and using only colour  $i$  and 0 (corresponding to the partition functions for the neighbourhood of  $v$  conditioned on  $\chi(v) = i$ ). Finally, let  $P_C^{(12)}(\lambda) = P_C^{(1)}(\lambda) + P_C^{(2)}(\lambda)$  and let

$$P_C(\lambda) = P_C^{(0)}(\lambda) + \lambda P_C^{(12)}(\lambda)$$

be the partition function of  $N(v) \cup \{v\}$  conditioned on the boundary conditions given by  $C$ . Note that if  $L$  has  $a_1$  lists containing 1 and  $a_2$  lists containing 2, then  $P_C^{(i)}(\lambda) = (1 + \lambda)^{a_i}$ .

Now we can write

$$(5) \quad \alpha^v(C) = \frac{\lambda P_C^{(12)}}{P_C} \quad \text{and} \quad \alpha^u(C) = \frac{\lambda \left( (P_C^{(0)})' + \lambda (P_C^{(12)})' \right)}{d P_C},$$

where  $P'$  is the derivative of  $P$  in  $\lambda$ . We will suppress the dependence of the partition functions on  $\lambda$  from now on.

For  $G = K_{d+1}$ , we have

$$P_{K_{d+1}} = 2(1 + \lambda)^{d+1} - 1$$

$$\alpha_{K_{d+1}}(\lambda) = \frac{2\lambda(1 + \lambda)^d}{2(1 + \lambda)^{d+1} - 1}.$$

If  $G = K_{d+1}$  then the only possible configuration is  $C_{K_{d+1}}$ , the complete neighbourhood  $K_d$  with full boundary lists, so we also have  $\alpha^u(K_d) = \alpha^v(K_d) = \alpha_{K_{d+1}}(\lambda)$  (we can also compute these directly). Since this quantity will arise frequently, we will use the notation  $\alpha_K = \alpha_{K_{d+1}}(\lambda)$ .

**2.2. A linear programming relaxation.** Now let  $q : \mathcal{C} \rightarrow [0, 1]$  denote a probability distribution over the set of all possible configurations. Then we set up the following optimisation problem over the variables  $q(C)$ ,  $C \in \mathcal{C}$ .

$$(6) \quad \alpha^* = \max \sum_{C \in \mathcal{C}} q(C) \alpha^v(C) \quad \text{subject to}$$

$$\sum_{C \in \mathcal{C}} q(C) = 1$$

$$\sum_{C \in \mathcal{C}} q(C) [\alpha^v(C) - \alpha^u(C)] = 0$$

$$q(C) \geq 0 \quad \forall C \in \mathcal{C}.$$

Note that this linear program is indeed a relaxation of our optimisation problem of maximising  $\alpha_G(\lambda)$  over all  $d$ -regular graphs: any such graph induces a probability distribution on  $\mathcal{C}$ , and as we have seen above in (4), the constraint asserting the equality  $\mathbb{E}\alpha^v(C) = \mathbb{E}\alpha^u(C)$  must hold in all  $d$ -regular graphs.

We will show that for any  $\lambda > 0$  the unique optimal solution of this linear program is  $q(C_{K_{d+1}}) = 1$ , where  $C_{K_{d+1}}$  is the configuration induced by  $K_{d+1}$ :  $H = K_d$  and  $L_u = \{1, 2\}$  for all  $u \in H$ .

The dual of the above linear program is

$$\alpha^* = \min \Lambda_p \quad \text{subject to}$$

$$\Lambda_p + \Lambda_c(\alpha^v(C) - \alpha^u(C)) \geq \alpha^v(C) \quad \forall C \in \mathcal{C},$$

with decision variables  $\Lambda_p$  and  $\Lambda_c$ .

To show that the optimum is attained by  $C_{K_{d+1}}$ , we must find a feasible solution to the dual program with  $\Lambda_p = \alpha_K = \frac{2\lambda(1+\lambda)^d}{2(1+\lambda)^{d+1}-1}$ . Note that with  $\Lambda_p = \alpha_K$  the constraint for  $C_{K_{d+1}}$  holds with equality for any choice of  $\Lambda_c$ . In other words, it suffices to find some convex

combination of the two local estimates  $\alpha^u$  and  $\alpha^v$  which is maximised by  $C_{K_{d+1}}$  over all  $C \in \mathcal{C}$ .

Let  $C_0$  be a configuration with  $L_u = \emptyset$  for all  $u \in H$  (in which case the edges of  $H$  are immaterial, and so abusing notation we will refer to any one of these configurations as  $C_0$ ). We find a candidate  $\Lambda_c$  by solving the constraint corresponding to  $C_0$  with equality:

$$\begin{aligned}\alpha_K &= \Lambda_c(\alpha^u(C_0) - \alpha^v(C_0)) + \alpha^v(C_0) \\ &= (1 - \Lambda_c) \frac{2\lambda}{1 + 2\lambda}.\end{aligned}$$

This gives

$$\Lambda_c = 1 - \frac{\alpha_K}{2\lambda}(1 + 2\lambda) = \frac{\alpha_K}{2\lambda} \frac{(1 + \lambda)^d - 1}{(1 + \lambda)^d}.$$

With this choice of  $\Lambda_c$ , the general dual constraint is

$$\alpha_K \geq \frac{\alpha_K}{2\lambda} \frac{(1 + \lambda)^d - 1}{(1 + \lambda)^d} \alpha^u(C) + \frac{\alpha_K}{2\lambda} (1 + 2\lambda) \alpha^v(C).$$

Using (5), this becomes

$$(7) \quad \frac{(P_C^{(0)})' + \lambda(P_C^{(12)})'}{2P_C^{(0)} - P_C^{(12)}} \leq \frac{d(1 + \lambda)^d}{(1 + \lambda)^d - 1}.$$

From this point on we may assume that  $C$  has some non-empty colour list, since otherwise the configuration is equivalent to  $C_0$  and the constraint holds with equality by our choice of  $\Lambda_c$ . This assumption tells us, among other things, that  $(P_C^{(0)})' > 0$  and  $2P_C^{(0)} - P_C^{(12)} > 0$ .

Our goal is now to show that (7) holds for all  $C$ . We consider the two terms separately.

**Claim 5.** *For any  $C \neq C_0$ ,*

$$\frac{\lambda(P_C^{(12)})'}{2P_C^{(0)} - P_C^{(12)}} \leq \frac{d\lambda(1 + \lambda)^{d-1}}{(1 + \lambda)^d - 1},$$

*with equality if and only if the lists  $L_u$  are all equal and  $C$  has no dichromatic colourings.*

*Proof.* Since the partition function  $P_C^{(0)}$  is at least the total weight  $P_C^{(1)} + P_C^{(2)} - 1$  of monochromatic colourings (with equality when  $C$  has no dichromatic colourings), we have

$$\frac{(P_C^{(12)})'}{2P_C^{(0)} - P_C^{(12)}} \leq \frac{(P_C^{(12)})'}{P_C^{(12)} - 2} = \frac{a_1(1 + \lambda)^{a_1-1} + a_2(1 + \lambda)^{a_2-1}}{(1 + \lambda)^{a_1} + (1 + \lambda)^{a_2} - 2}$$

(where, as above,  $a_i$  is the number of vertices in  $H$  allowed colour  $i$  under the given boundary conditions), and so we need to show that

$$(8) \quad \frac{a_1(1 + \lambda)^{a_1-1} + a_2(1 + \lambda)^{a_2-1}}{(1 + \lambda)^{a_1} + (1 + \lambda)^{a_2} - 2} \leq \frac{d(1 + \lambda)^{d-1}}{(1 + \lambda)^d - 1}.$$

In general, to show that  $(a + b)/(c + d) \leq t$  it suffices to show that  $a/c \leq t$  and  $b/d \leq t$ . Thus it is enough to show that

$$(9) \quad \frac{a(1 + \lambda)^{a-1}}{(1 + \lambda)^a - 1} \leq \frac{d(1 + \lambda)^{d-1}}{(1 + \lambda)^d - 1}$$

whenever  $1 \leq a \leq d$ . (Note that if either  $a_1 = 0$  or  $a_2 = 0$  then (8) reduces to (9), and if both  $a_1, a_2 = 0$  then the configuration is  $C_0$ ). Indeed, it is not hard to check via calculus that the left hand side of (9) is increasing with  $a$ . This completes the proof of the inequality in Claim 5.

We have equality in this final step when  $a_1 = a_2 = d$  or when one is 0 and the other is  $d$ . So we have equality overall whenever the lists are all equal and there are no dichromatic colourings (recall that we are assuming  $C$  has some non-empty colouring list).  $\square$

**Claim 6.** *For any  $C \neq C_0$ ,*

$$\frac{(P_C^{(0)})'}{2P_C^{(0)} - P_C^{(12)}} \leq \frac{d(1+\lambda)^{d-1}}{(1+\lambda)^d - 1},$$

*with equality if and only if the lists  $L_u$  are all equal and  $C$  has no dichromatic colourings.*

*Proof.* We can write

$$\begin{aligned} \frac{\lambda(P_C^{(0)})'}{2P_C^{(0)} - P_C^{(12)}} &= \frac{\lambda(P_C^{(0)})'}{P_C^{(0)}} \cdot \frac{P_C^{(0)}}{(P_C^{(0)} - P_C^{(1)}) + (P_C^{(0)} - P_C^{(2)})} \\ &= \frac{\mathbb{E}_C[X_1] + \mathbb{E}_C[X_2]}{\mathbb{P}_C[X_1 > 0] + \mathbb{P}_C[X_2 > 0]}, \end{aligned}$$

where now  $X_i$  is the number of vertices coloured  $i$  in a random colouring chosen from the Widom–Rowlinson model on  $C$ . Noting that  $\mathbb{E}_C[X_1] = 0$  whenever  $\mathbb{P}_C[X_1 > 0] = 0$ , it suffices as above to show that whenever colour 1 is permitted anywhere in  $C$ ,

$$(10) \quad \frac{\mathbb{E}_C[X_1]}{\mathbb{P}_C[X_1 > 0]} = \mathbb{E}_C[X_1 \mid X_1 > 0] \leq \frac{\lambda d(1+\lambda)^{d-1}}{(1+\lambda)^d - 1} = \mathbb{E}_{K_d}[X_1 \mid X_1 > 0],$$

and similarly for  $X_2$ , but this will follow by symmetry.

We can decompose the expectation as

$$\mathbb{E}_C[X_1 \mid X_1 > 0] = \sum_{S \subseteq V(H)} \mathbb{P}_C[\chi^{-1}(2) = S \mid X_1 > 0] \cdot \mathbb{E}_C[X_1 \mid X_1 > 0 \wedge \chi^{-1}(2) = S].$$

The partition function restricted to colourings satisfying  $X_1 > 0$  and  $\chi^{-1}(2) = S$  is just  $P_S(\lambda) = \lambda^{|S|}((1+\lambda)^{a_S} - 1)$ , where  $a_S$  is the number of vertices in  $H \setminus S$  which are allowed colour 1 and are not adjacent to any vertex of  $S$ . The conditional expectation is then

$$\mathbb{E}_C[X_1 \mid X_1 > 0 \wedge \chi^{-1}(2) = S] = \frac{a_S \lambda (1+\lambda)^{a_S-1}}{(1+\lambda)^{a_S} - 1} \leq \frac{d \lambda (1+\lambda)^{d-1}}{(1+\lambda)^d - 1}$$

with equality precisely when  $S$  is empty and 1 is available for every vertex. That is,

$$\mathbb{E}_C[X_1 \mid X_1 > 0] \leq \sum_{S \subseteq V(H)} \mathbb{P}_C[\chi^{-1}(2) = S \mid X_1 > 0] \cdot \frac{d \lambda (1+\lambda)^{d-1}}{(1+\lambda)^d - 1} = \frac{\lambda d (1+\lambda)^{d-1}}{(1+\lambda)^d - 1},$$

as desired. We have equality in (10) when  $\mathbb{P}_C[a_S = d \mid X_1 > 0] = 1$ , which holds for the configurations where 1 is available to every vertex but which have no dichromatic colourings. That is, for equality to hold in the claim  $C$  must have no dichromatic colourings, and any colour which is available to some vertex  $u$  must be available to every vertex (so the lists must be identical).  $\square$



Adding the inequalities in Claims 6 and 5 shows that (7) holds for all  $C$ , proving optimality of  $K_{d+1}$ .

### 2.3. Uniqueness.

**Lemma 7.** *The distribution induced by  $K_{d+1}$  is the unique optimum of the LP relaxation (6).*

*Proof.* Complementary slackness for our dual solution says that any optimal primal solution is supported only on configurations  $C$  with identical boundary lists and no dichromatic colourings. These fall into three categories:

**Case 0:**  $L_u = \emptyset$  for all  $u$ . In this case the edges of  $H$  are immaterial, as none of  $H$  can be coloured. This is the configuration  $C_0$  above.

**Case 1:**  $L_u = \{i\}$  for all  $u$  (for  $i = 1$  or  $2$ ). The edges of  $H$  are again immaterial, as every colouring of  $H$  with only colour  $i$  is allowed. Call this configuration  $C_1$ .

**Case 2:**  $L_u = \{1, 2\}$  for all  $u$ . In this case the prohibition on dichromatic colourings requires that  $C = C_{K_{d+1}}$ .

We can calculate  $\alpha^v(C)$  and  $\alpha^u(C)$  for each case. For Case 0 we have

$$\alpha^v(C_0) = \frac{2\lambda}{1+2\lambda} \quad \text{and} \quad \alpha^u(C_0) = 0.$$

For Case 1 we have

$$\alpha^v(C_1) = \frac{\lambda + \lambda(1+\lambda)^d}{\lambda + (1+\lambda)^{d+1}} \quad \text{and} \quad \alpha^u(C_1) = \frac{\lambda(1+\lambda)^d}{\lambda + (1+\lambda)^{d+1}}.$$

And of course, for Case 2 we have

$$\alpha^v(K_d) = \alpha^u(K_d) = \alpha_K.$$

In both Case 0 and Case 1 we have  $\alpha^u < \alpha^v$ , so the only convex combination  $q$  of the three cases giving  $\sum_C q(C)\alpha^u(C) = \sum_C q(C)\alpha^v(C)$  (as is required for feasibility) is the one which puts all of the weight on  $C_{K_{d+1}}$ .  $\square$

### 3. DISTINCT ACTIVITIES

It is also natural to consider a weighted version of the Widom–Rowlinson model with distinct activities  $\lambda_1, \lambda_2$  for the two colours, so that the configuration  $\chi$  is chosen according to the distribution

$$\mathbb{P}[\chi] = \frac{\lambda_1^{X_1(\chi)} \lambda_2^{X_2(\chi)}}{P_G(\lambda_1, \lambda_2)}$$

where the partition function is

$$P_G(\lambda_1, \lambda_2) = \sum_{\chi \in \Omega(G)} \lambda_1^{X_1(\chi)} \lambda_2^{X_2(\chi)}.$$

We can ask which  $d$ -regular graphs maximise  $P(\lambda_1, \lambda_2)^{1/|V(G)|}$ .

**Conjecture 8.** *For any  $\lambda_1, \lambda_2 > 0$ , and any  $d$ -regular graph  $G$ ,*

$$(11) \quad P_G(\lambda_1, \lambda_2) \leq P_{K_{d+1}}(\lambda_1, \lambda_2)^{|V(G)|/(d+1)}.$$

Now denote by  $\alpha_G^1(\lambda_1, \lambda_2)$  and  $\alpha_G^2(\lambda_1, \lambda_2)$  the expected fraction of vertices of  $G$  that receive colours 1 and 2 respectively in this model.

**Conjecture 9.** *For any  $\lambda_1, \lambda_2 > 0$ , the weighted occupancy fraction*

$$\bar{\alpha}_G(\lambda_1, \lambda_2) = \frac{\lambda_2 \alpha_G^1(\lambda_1, \lambda_2) + \lambda_1 \alpha_G^2(\lambda_1, \lambda_2)}{\lambda_1 + \lambda_2}$$

*is maximised over all  $d$ -regular graphs by  $K_{d+1}$ .*

In fact, Conjecture 9 implies Conjecture 8. To see this, assume  $\lambda_1 \geq \lambda_2$ , and let  $F_G(x) = \frac{1}{n} \log P_G(\lambda_1 - \lambda_2 + x, x)$ . We have

$$\frac{1}{n} \log P_G(\lambda_1, \lambda_2) = F_G(\lambda_2) = F_G(0) + \int_0^{\lambda_2} \frac{dF_G}{dx}(x) dx$$

$F_G(0) = \frac{1}{n} \log P_G(\lambda_1 - \lambda_2, 0) = \log(1 + \lambda_1 - \lambda_2)$  for all graphs  $G$ , and so if we can show that for all  $0 \leq x \leq \lambda_2$ ,  $\frac{dF_G}{dx}(x)$  is maximised when  $G = K_{d+1}$ , then we obtain (the log of) inequality (11). We compute:

$$\begin{aligned} \frac{dF_G}{dx}(x) &= \frac{1}{n} \frac{\frac{d}{dx} P_G(\lambda_1 - \lambda_2 + x, x)}{P_G(\lambda_1 - \lambda_2 + x, x)} \\ &= \frac{1}{n} \frac{\sum_X \frac{x X_1 + (\lambda_1 - \lambda_2 + x) X_2}{x(\lambda_1 - \lambda_2 + x)} (\lambda_1 - \lambda_2 + x)^{X_1} \cdot x^{X_2}}{P_G(\lambda_1 - \lambda_2 + x, x)} \\ &= \frac{1}{x(\lambda_1 - \lambda_2 + x)} \frac{1}{n} \frac{\sum_X (x X_1 + (\lambda_1 - \lambda_2 + x) X_2) (\lambda_1 - \lambda_2 + x)^{X_1} \cdot x^{X_2}}{P_G(\lambda_1 - \lambda_2 + x, x)} \\ &= \frac{1}{x(\lambda_1 - \lambda_2 + x)} \left[ x \alpha_G^{(1)}(\lambda_1 - \lambda_2 + x, x) + (\lambda_1 - \lambda_2 + x) \alpha_G^{(2)}(\lambda_1 - \lambda_2 + x, x) \right]. \end{aligned}$$

Conjecture 9 implies that this is maximised by  $K_{d+1}$ .

## REFERENCES

- [1] G. Brightwell and P. Winkler. Hard constraints and the Bethe lattice: adventures at the interface of combinatorics and statistical physics. In *Proc. Int'l. Congress of Mathematicians*, volume III, pages 605–624, 2002.
- [2] J. Chayes, L. Chayes, and R. Kotecký. The analysis of the Widom–Rowlinson model by stochastic geometric methods. *Communications in Mathematical Physics*, 172(3):551–569, 1995.
- [3] E. Davies, M. Jenssen, W. Perkins, and B. Roberts. Independent sets, matchings, and occupancy fractions. *arXiv preprint arXiv:1508.04675*, 2015.
- [4] A. Dembo, A. Montanari, N. Sun, et al. Factor models on locally tree-like graphs. *The Annals of Probability*, 41(6):4162–4213, 2013.
- [5] D. Galvin. Maximizing  $H$ -colorings of a regular graph. *Journal of Graph Theory*, 73(1):66–84, 2013.
- [6] D. Galvin. Three tutorial lectures on entropy and counting. *arXiv preprint arXiv:1406.7872*, 2014.
- [7] D. Galvin and P. Tetali. On weighted graph homomorphisms. *DIMACS Series in Discrete Mathematics and Theoretical Computer Science*, 63:97–104, 2004.
- [8] J. Kahn. An entropy approach to the hard-core model on bipartite graphs. *Combinatorics, Probability and Computing*, 10(03):219–237, 2001.
- [9] J. Lebowitz and G. Gallavotti. Phase transitions in binary lattice gases. *Journal of Mathematical Physics*, 12(7):1129–1133, 1971.
- [10] J. Radhakrishnan. Entropy and counting. *Computational Mathematics, Modelling and Algorithms*, page 146, 2003.
- [11] D. Ruelle. Existence of a phase transition in a continuous classical system. *Physical Review Letters*, 27(16):1040, 1971.

- [12] L. Sernau. Graph operations and upper bounds on graph homomorphism counts. *arXiv preprint arXiv:1510.01833*, 2015.
- [13] B. Widom and J. S. Rowlinson. New model for the study of liquid–vapor phase transitions. *The Journal of Chemical Physics*, 52(4):1670–1684, 1970.
- [14] Y. Zhao. The number of independent sets in a regular graph. *Combinatorics, Probability and Computing*, 19(02):315–320, 2010.
- [15] Y. Zhao. The bipartite swapping trick on graph homomorphisms. *SIAM Journal on Discrete Mathematics*, 25(2):660–680, 2011.

SCHOOL OF MATHEMATICS, GEORGIA INSTITUTE OF TECHNOLOGY

*E-mail address:* `ecohen32@gatech.edu`

SCHOOL OF MATHEMATICS, UNIVERSITY OF BIRMINGHAM

*E-mail address:* `math@willperkins.org`

SCHOOL OF MATHEMATICS, GEORGIA INSTITUTE OF TECHNOLOGY

*E-mail address:* `tetali@math.gatech.edu`